

Numerical modeling of the influence of the electric field and the concentration of traps on the capture of diffusing particles in spaces of different dimensions (one-dimensional, two-dimensional and three-dimensional)

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Abstract

Numerical simulations of particle diffusion in media with absorbing traps under an applied electric field were performed. The results demonstrate that, over sufficiently long timescales, the drift mechanism governs the novel temporal behavior of the survival probability. The dependences of the characteristic time describing the exponential decay of the particle population on trap concentration and electric field strength were determined.

Introduction

The problem of particle diffusion in media with absorbing traps has been extensively investigated [1–3]. Interest in this topic stems from its numerous applications, as well as its analogy to the density of states problem in disordered media [4] and its implications for novel particle transport phenomena [5]. In [6], the capture of randomly distributed diffusing particles by absorbing traps was examined in detail. It was shown that the particle survival probability $W(t, C)$ decays exponentially at short times $t \ll t_c$, where $t_c = (DC^2)^{-1}$, (with D being the diffusion coefficient and C the trap concentration in the one dimensionion):

$$W(t, C) \propto W_0 \exp\left(-\frac{t}{t_c}\right)$$

(1)

However, at large times, the asymptotics of the survival probability is determined by the existence of sufficiently large regions free of absorbing traps, and is of a fractional-exponential nature:

$$W(t, c) \propto W_0 \left(\frac{Dtc^2}{3\pi} \right)^{1/2} \exp \left(- \frac{3\pi^{1/2} (Dtc^2)^{1/3}}{2} \right) \quad (2)$$

The influence of a drift transport mechanism on particle dynamics was previously studied in [7-9]. It was demonstrated that, over sufficiently long timescales, drift determines the temporal asymptotics of the survival probability in media with absorbing traps.

When incorporating an electric field into the diffusion problem with absorbing traps, two new parameters arise. The first is the "field" time, the time at which the drift displacement is compared to the diffusion displacement: $v^2 t_E^2 \propto Dt_E$ (v is the particle's drift velocity):

$$t_E = \frac{v^2}{D} \quad (3)$$

It's easy to see that at times longer than the "field" drift, particle drift becomes dominant. Accordingly, in sufficiently strong fields, a new asymptotic behavior was predicted for the probability of particle survival in media with absorbing traps, with a characteristic time dependent on the electric field strength. The second dimensionless parameter is also related to drift in the electric field and is equal to the ratio of potential energy to temperature.

$$\frac{v l}{D} = \frac{qEl}{kT} \quad (4)$$

This expression follows directly from the Einstein relation $\mu kT = D$, where μ is the particle mobility, ($v = \mu E$), kT is the thermal energy.

The introduction of an electric field into the diffusion-with-traps problem not only alters the time dependence of the survival probability but also raises the question of possible field-induced phase transitions, specifically a transition from localization within trap-rich regions to long-time drift under the field's influence [10-12]. According to existing results, a critical field E_c exists. For fields below this threshold $E \ll E_c$, the average particle drift velocity is zero $V=0$, whereas for $E > E_c$ a non-zero average drift velocity $V>0$ emerges [13-16].

In this work, we perform numerical simulations of diffusion processes in media with traps under an applied electric field. We investigate the dependence of the effective decay time of the survival probability on electric field strength and trap concentration for one-, two-, and three-dimensional systems. This dependence is visualized as a two-dimensional surface.

The article is structured as follows. Section 2 outlines the key theoretical results concerning the influence of an electric field on particle trapping. Section 3 details the simulation algorithm and methodology, including result visualization. Section 4 presents the numerical simulation results. The Conclusion discusses the findings and their implications.

2. Diffusion in Media with Traps. Effect of an Electric Field on Particle Capture.

We briefly summarize the principal arguments leading to result (1) for diffusion in media with traps. Following [5], a solution to the standard diffusion equation is constructed:

(5)

with the following initial and boundary conditions:

$$W(x, 0) = \frac{1 - C}{L}, \quad W(x_i, t) = W(x_{i+1}, t) = 0$$

(6)

Here L is the system length, x_i, x_{i+1} are the coordinates of the absorbing traps. The solution takes the form:

$$W(x, t; x_i) = \frac{4}{L} \sum_{n=0}^{\infty} \exp\left(-\frac{Dk_n^2 t}{2}\right) \frac{\sin(k_n(x - x_i))}{k_n l_i}$$

(7)

where $k_n = \frac{(2n+1)\pi}{l_i}$, $l_i = |x_{i+1} - x_i|$

The quantity of interest is the survival probability $W(x, t; \bar{W}(t))$ obtained by averaging over all trap intervals:

$$\bar{W}(t) = \sum_i W(t, x_i) = \sum_i \int_{x_i}^{x_{i+1}} W(x, t; x_i) dx$$

(8)

For a random Poisson distribution of traps $f(l) = c \exp(-cl)$,

where $c = \frac{N}{L}$ is where is the concentration of traps, l is the distance between traps, we obtain formula (1) for short periods of time, and formula (2) for long periods of time.

2.1. Influence of an Electric Field on the Survival Probability in Media with Traps

The electric field is incorporated into the diffusion problem in the standard manner, leading to the drift-diffusion equation:

$$\frac{\partial \mathcal{W}(x, t)}{\partial t} = D \frac{\partial^2 \mathcal{W}(x, t)}{\partial x^2} + v \frac{\partial \mathcal{W}(x, t)}{\partial x}$$

(9)

Here $v = \mu E$ is the drift velocity of particles in an electric field E , μ and is the particle mobility. We set the initial and boundary conditions similar to those formulated above (6). Accordingly, we seek a solution in the form of an expansion in eigenfunctions:

(11)

and the eigenvalues are determined by the expression:

$$E_n = Dk_n^2 + \frac{v^2}{4D}$$

(12)

Accordingly, in times $t \gg t_E$ we obtain an exponential decrease due to the drift of particles onto absorbing traps under the influence of an electric field, corresponding to the mean field approximation

$$\overline{\mathcal{W}}(t, E) \propto \exp\left(-\frac{v^2 t}{4D}\right)$$

(13)

2.2. Effect of Trap Concentration Fluctuations and Electric Field on the Fluctuation Mechanism

According to the results of [7-9], the asymptotic solution depends the electric field strength. For weak fields (or small scales) satisfying $\frac{v l}{D} \ll 1$, the well-known result holds: the survival probability is governed by fluctuations in trap concentration, i.e., the existence of large trap-free regions, as given by formula (2). In the opposite limit of strong fields, a new asymptotic behavior arises:

$$\mathcal{W}(t, E) \propto W_0 \exp\left(-\frac{v^2}{4D} t - \frac{3\pi^{1/2} \left(D t^{1/3} \left[1 + \frac{qE}{4ckT} \right] \right)^{1/3}}{2}\right)$$

(14)

Thus, on large scales and/or in strong electric fields, the long-time survival probability is determined by a combination of field-driven drift (first term in the exponential) and drift over distances comparable to the mean inter-trap separation, modified by concentration fluctuations (second term).

2.3. Average Drift Velocity and Phase Transitions

2.3.1. Short-Time Asymptotics in the Effective Medium Approximation.

Introducing an electric field leads to the possibility of field-induced phase transitions, specifically a transition from localization within trap regions to long-time drift [10-12]. To determine the average drift velocity, we compute the first moment of the solution to the diffusion equation:

$$\langle X \rangle = \sum_{i=1}^{\infty} \int_{x_i}^{x_{i+1}} (x - x_i) W(x, t | E) dx \quad (10)$$

Averaging over trap positions using the distribution function $f(l)$ yields:

$$\langle X \rangle = \langle l \rangle + v \frac{C_1 \langle l^2 \rangle}{C_2 \langle l \rangle} \quad (11)$$

Here C_1 and C_2 are numerical coefficients and moments are determined by the expression: $\langle l^k \rangle = \int_0^{\infty} l^k \exp\left(-\frac{Dt}{l^2}\right) f(l) dl$

In the effective medium approximation, this trap distribution function is equal to: $f(l) = \exp(-cl^2)$:

For the one-dimensional case:

$$\langle X \rangle = c^1 + C_3 v t_c \quad (12)$$

where C_3 the constant coefficient and $t_c = 1/Dc^2$ is the diffusion time for the average distance between traps. Since the mean displacement becomes finite and time-independent, the average drift velocity in this approximation is zero:

$$\langle V \rangle = \frac{d\langle X \rangle}{dt} = 0 \quad (13)$$

This result, consistent with previous studies [13-16], has a clear physical basis: particles undergo brief motion between traps before being captured, leading to a finite mean displacement and zero net drift velocity. The effective medium approximation is valid for short times $t \ll t_c$; hence, result (16) corresponds to complete localization on these timescales.

2.3.2. Long-Time Asymptotics in the Effective Medium Approximation

For long times, determined by the existence of rare regions free of traps, the temporal asymptotics of particle survival due to fluctuations yields a different, new time dependence of the average drift velocity. Using formula (11) above, it is necessary to calculate the moments $\langle l^n \rangle$. For a Poisson random distribution of traps and the one-dimensional case $f(l) = c \exp(-cl)$, where $c = N/l$ is the trap concentration, these moments are equal to:

$$\begin{aligned} \langle l^1 \rangle &= \int_0^\infty l \exp\left(-\frac{Dt}{l^2} - cl\right) dl \propto t^{1/3} \\ \langle l^2 \rangle &= \int_0^\infty l^2 \exp\left(-\frac{Dt}{l^2} - cl\right) dl \propto t^{2/3} \end{aligned} \quad (14)$$

These moments were calculated using the saddle-point method. This yields an expression for the first moment of the Green's function of random motion in weak electric fields and over long periods of time:

$$\langle X \rangle \propto v t_c^{1/3} t^{2/3} \quad (15)$$

Thus, the average drift velocity in the weak fields under consideration and over large times is equal to:

$$\langle V \rangle = \frac{d\langle X \rangle}{dt} \propto v \left(\frac{t_c}{t} \right)^{1/3} \quad (16)$$

The main feature of formula (16) is the dependence of the average velocity on time. This dependence is analogous to the case of subdiffusive random walks [17]. Therefore, we can introduce the concept of "subdrift" behavior—a decrease in the average effective velocity of diffusing particles due to the capture and subsequent loss of particles. However, this effective velocity also asymptotically tends to zero. Thus, we can speak of quasi-localization at large times. To test the developed theoretical concepts, numerical simulations were conducted.

3. Numerical Simulation of the Effect of an Electric Field on Particle Capture.

The objective of this numerical study is to investigate particle dynamics in one-, two-, and three-dimensional media with absorbing traps under an applied electric field. The simulation aims to analyze particle distributions, establish the asymptotic behavior of the survival probability, and examine the influence of field strength and trap

concentration on these asymptotics. Specifically, we focus on the role of field-induced drift transport in determining particle survival upon encounter with traps. The model incorporates parameters affecting particle motion: electric field direction and magnitude; interparticle interactions; trap locations; and initial conditions. This parameter set allows simulation of a system where the electric field induces drift transport toward absorbing traps, thereby enhancing particle absorption.

Model: algorithm and implementation.

Particle motion is simulated using a random walk model with discrete steps along the coordinate axes, incorporating the influence of a constant, uniform electric field. The field introduces a directional bias, increasing the probability of motion along the field direction. Key aspects of the simulation algorithm include system initialization, the particle motion routine, and absorption checking.

The implementation is in C++ for high performance. A Mersenne Twister random number generator ensures high-quality stochastic sequences. Parallelization via OpenMP accelerates computations by distributing independent simulation runs across multiple threads. System parameters (particle density, field strength, etc.) are configurable via input files. The code structure permits straightforward modification of interaction rules, such as introducing new trap types or adjusting field-response dynamics.

Data Visualization and Analysis

The following techniques were employed for analysis and visualization:

- Particle trajectory plots (2D/3D) to track positional changes and field influence.
- Density heat maps to identify particle clustering and regions of impeded motion.
- Graphs of movement probability over time to quantify field and trap concentration effects.

All visualizations were generated using custom Python scripts.

4. Simulation results.

Results for systems of different dimensionality are presented below.

4.1. One-dimensional case.

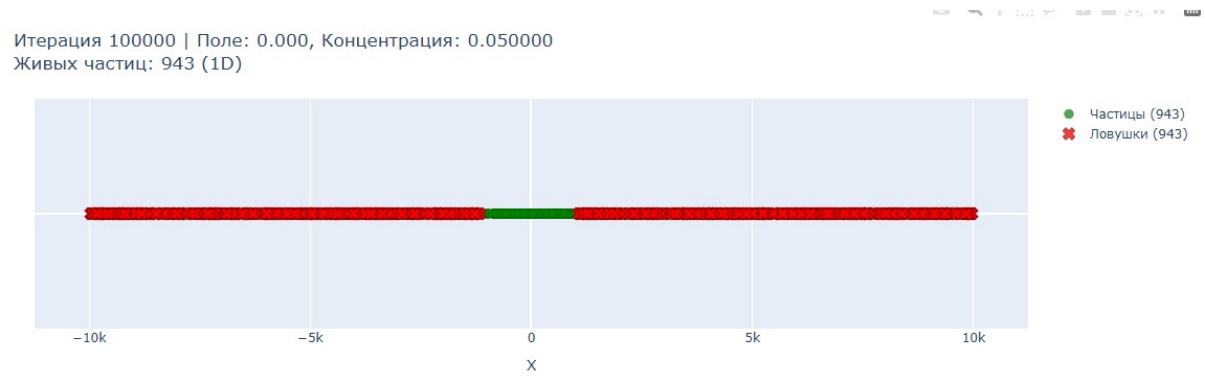


Fig. 1a) Diffusion along a segment with traps. $t = 100,000$. Trap concentration $c = 0.05$; they are colored red.

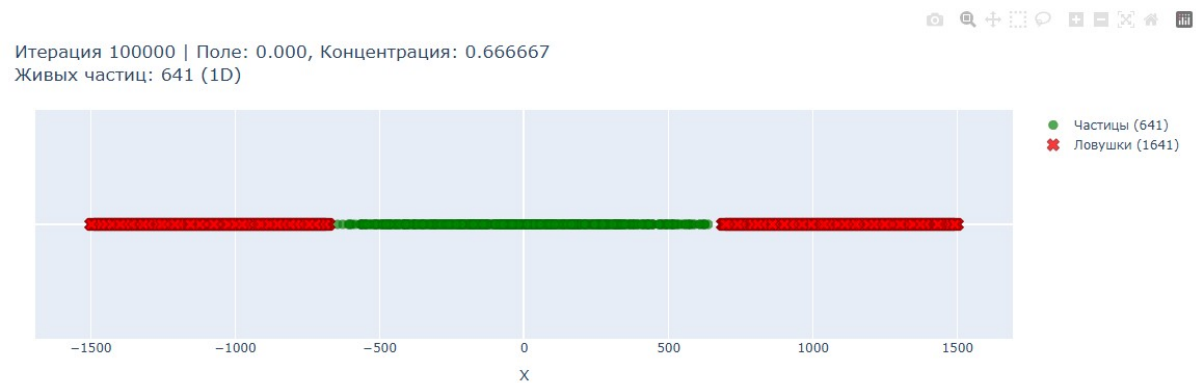


Fig. 1b) Diffusion along a segment with traps. $t = 100,000$ in a medium with a higher concentration of traps, $c = 0.66667$

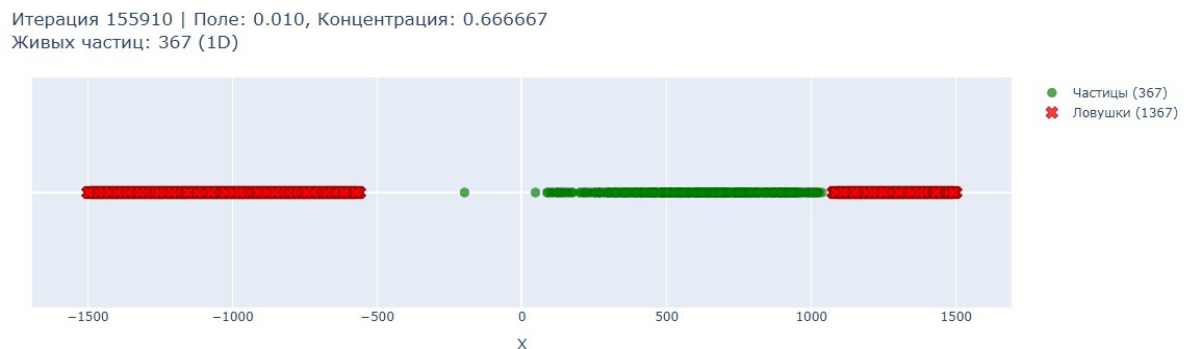


Fig. 1c) Diffusion in an electric field - particle displacement to the right along the field $t = 155910$, $c = 0.666667$, anisotropy $E = 0.01$

The graphs show obvious diffusional spreading of particles and a decrease in the density of traps in the center due to their filling with diffusing particles; when the field is turned on, the particles begin to shift along the field (to the right).

As a result of the simulation, we obtain the following functional dependence of the lifetime on the concentration and electric field (Fig. 2).

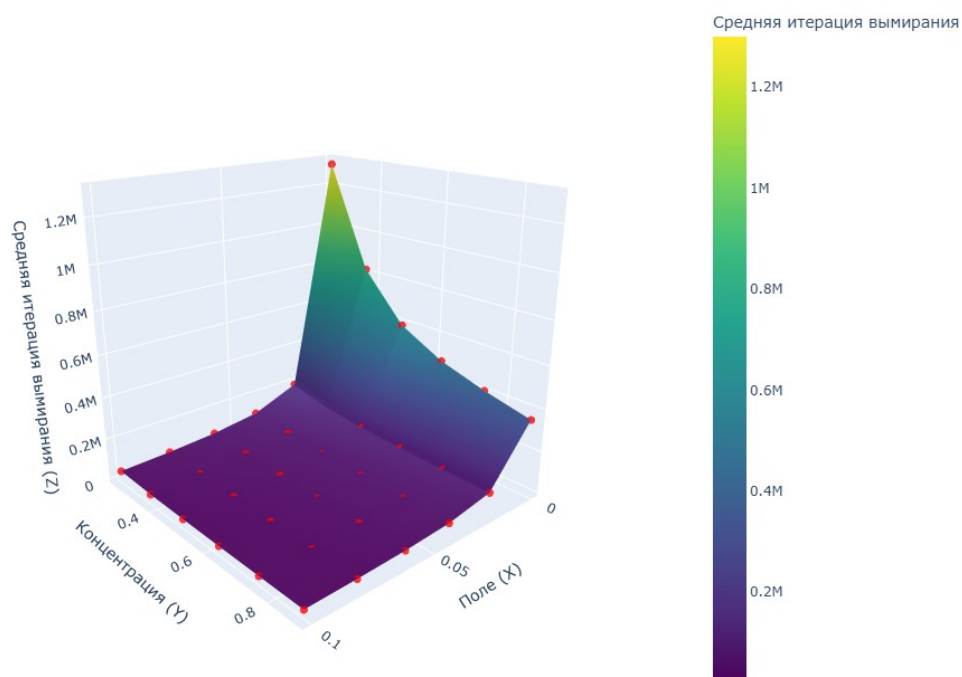


Fig. 2. Dependence of lifetime on concentration and magnitude of electric field in the one-dimensional case.

4.2. Two-dimensional case.

The two-dimensional case was previously analyzed in detail in our article [18] for rectangular regions. This article presents the calculation results for the location and traps inside the circle.

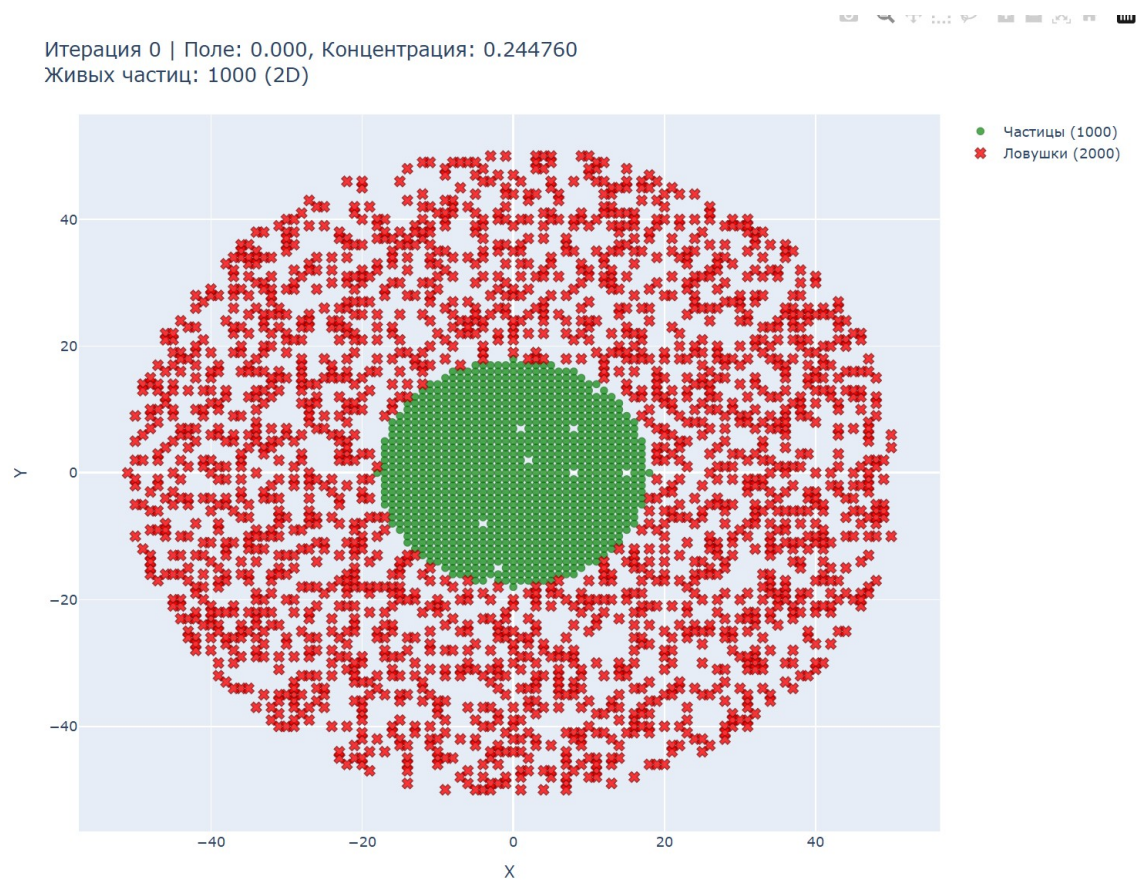


Fig. 3a) Initial distribution of particles (green). Concentration of traps $c=0.244760$, they are colored red.

Итерация 657 | Поле: 0.000, Концентрация: 0.244760
Живых частиц: 367 (2D)

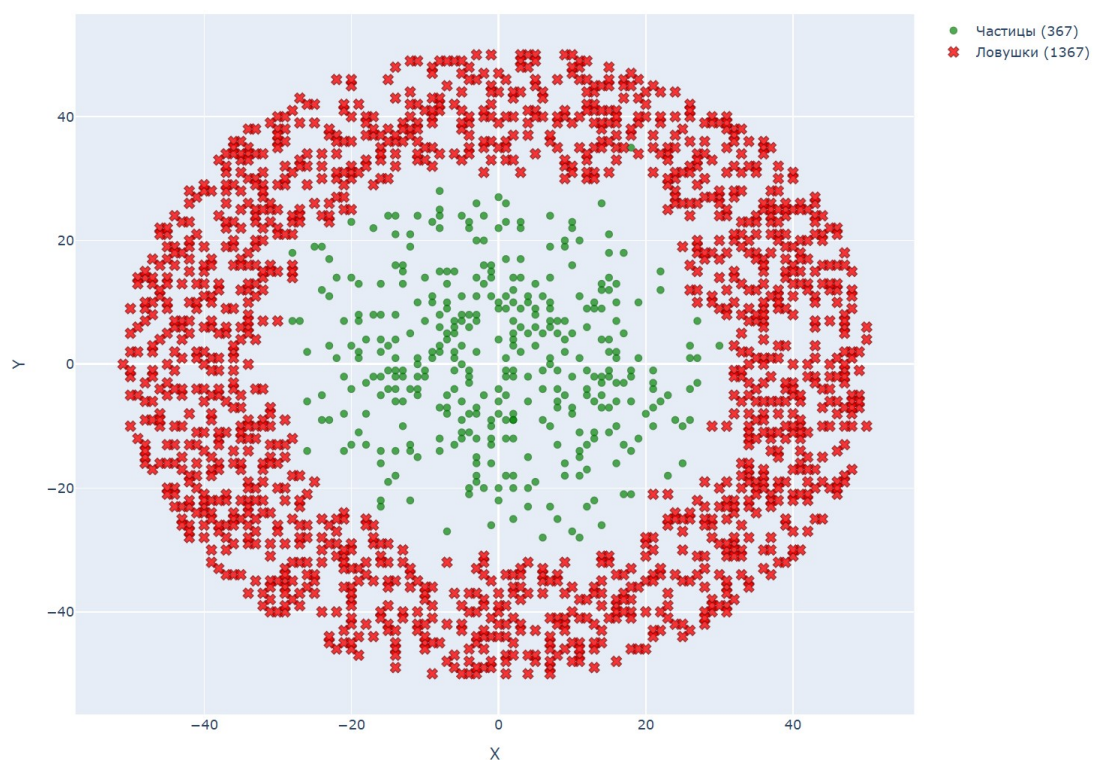


Fig. 3b) Diffusion of particles (green) inside the circle; concentration of traps (red) $c=0.244760$. The process of intense absorption of particles by traps is reflected

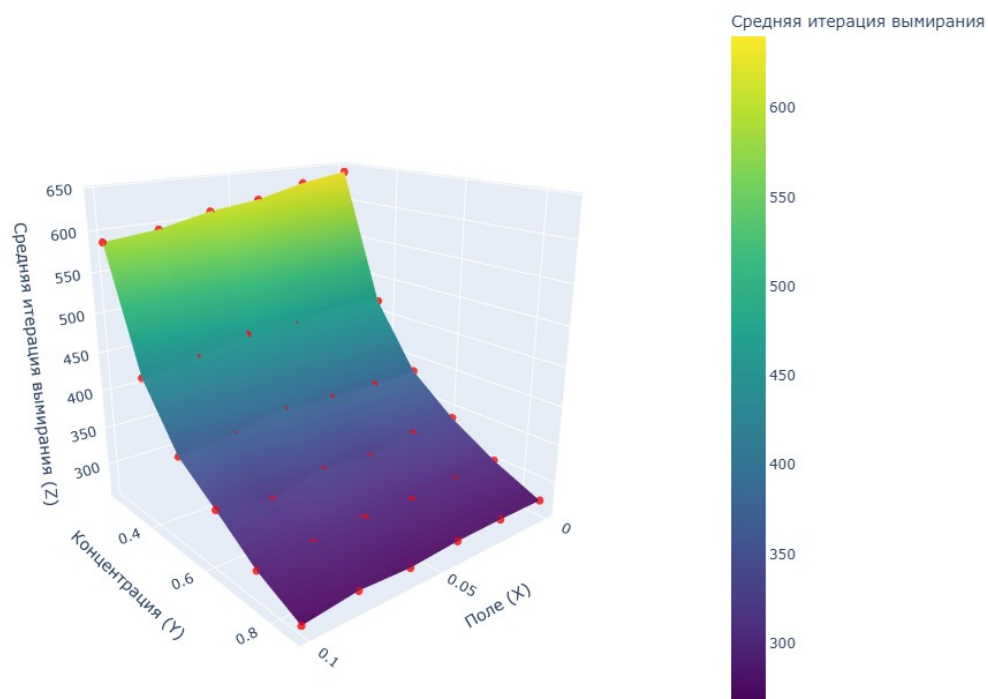


Fig. 4. Dependence of lifetime on concentration and electric field strength in the two-dimensional case.

4.3. Three-dimensional case

Numerical modeling of particle capture in three-dimensional traps is not significantly different from the two-dimensional case, since in both cases, particles have the opportunity to avoid capture, unlike in the one-dimensional case, where particles inevitably fall into traps and are captured. The obtained results for the effective decay time can be more clearly represented as a function of two variables.

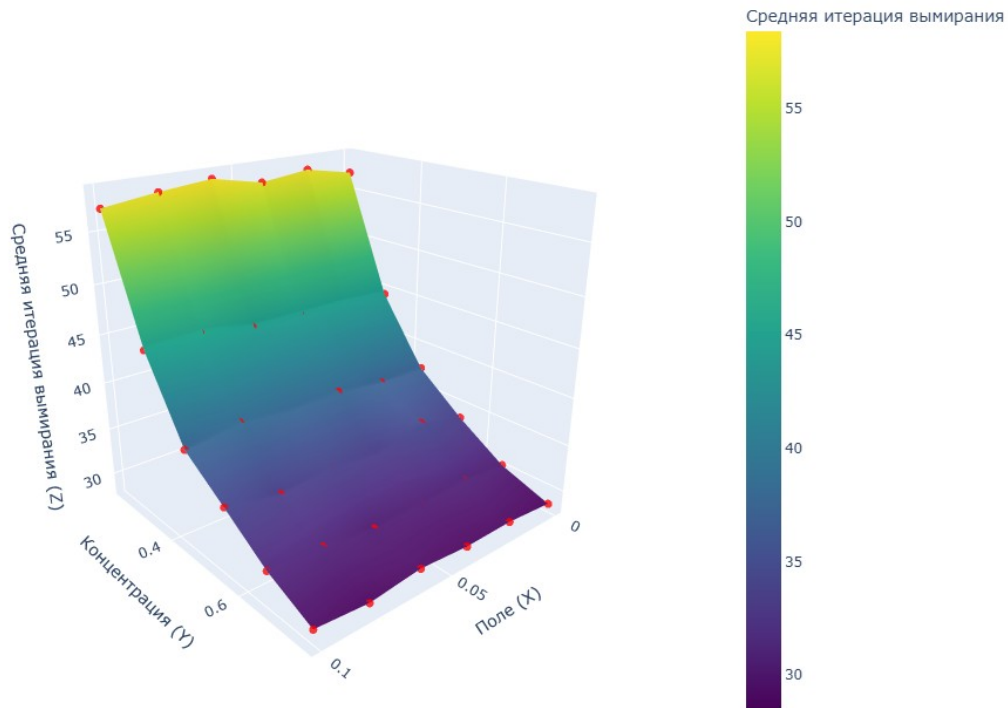


Fig. 5. Dependence of the lifetime on the concentration and magnitude of the electric field.

Let us discuss the physical meaning of the obtained results and their analogy with phase transitions. According to our results, there is a sharp transition from particle localization between traps, i.e., a transition from a state with zero average velocity to a state with subdrift—with an average effective velocity that decreases over time. This transition has the form of a second-order phase transition, since the velocity changes continuously.

The obtained numerical simulation results show a significant difference between diffusion in an electric field in the one-dimensional case and diffusion in higher-dimensional media—two- and three-dimensional ones. A stronger dependence on diffusion anisotropy is evident in the one-dimensional case—see Fig. 2 and Fig. 4.

5. Conclusion.

Thus, in this article, we investigated the problem of diffusing particle trapping in an electric field using numerical simulation methods. We established the asymptotic time dependences of particle survival in spaces of different dimensions—one-, two-, and three-dimensional—and the

influence of two parameters—the trap concentration and the electric field strength—on these asymptotics.

Since diffusion problems involve only two characteristic times and, accordingly, two parameters, we can therefore assume a self-similar solution to the problem of diffusing particle trapping in an electric field, namely, the logarithm of the particle survival probability $\ln(W(x, y)/W_0) = -f(x, y)$:

$$f(x, y) \propto x^{1/3} g\left(\frac{y}{x}\right) = \begin{cases} x^{1/3}, & 1 \ll x, y \ll 1 \\ Ay^{1/3}, & 1 \ll x \ll y \end{cases}$$

(17)

According to the scaling approach, in weak electric fields, the function depends only on the current time and the trapping time $t_c = (Dc^2)^{-1}$, i.e., only on the parameter x , in a power-law fashion—the upper asymptotics of formula (16). In the case of strong electric fields, when the "field" length $L_E = kT/qE$ becomes smaller than the distance between traps $L_c = 1/c$: $L_c \ll L_E$ or, in terms of the electric field $1 \ll qE/kTc$, we obtain a dependence only on the parameter y —the lower asymptotics of formula (16).

The numerical simulation of the processes of diffusing particle capture in traps and the influence of an electric field confirms the feasibility of using a scaling approach for the problems under study. However, there is a certain asymmetry depending on the parameters, namely, a slower decrease in the effective time with increasing electric field; this difference is particularly noticeable in the one-dimensional case. This is easy to understand, since in the one-dimensional case, the existence of even a single trap is critical for the particle dynamics.

Acknowledgments

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Appendix A. Description of the Model and Numerical Simulation Algorithm.

Model parameters that directly affect particle motion:

- Electric field direction and intensity: The electric field exerts a directional force on particles, causing them to move more frequently toward the field. To achieve this, a constant shift, describing the effect of the electric field, is added to the random particle movements.
- Particle interactions in space: Particles neither attract nor repel each other, but cannot occupy the same location simultaneously. If two particles attempt to move to the same point, they return to their original positions.

This constraint simulates the "repulsion" that occurs when attempting to intersect in space.

- Traps: Traps are randomly placed in space; they absorb any particle that enters them. Entering a trap results in the complete disappearance of the particle from the system. The locations of the traps remain fixed throughout the simulation, allowing one to study the effect of traps on particle survival.
- Initial conditions: The initial positions of particles and traps determine their initial arrangement. The density and distribution of traps, as well as the initial positions of particles, are specified to explore various scenarios of interaction with traps and drift displacement under the influence of the field.

This set of parameters allows us to simulate a system in which an electric field creates drift transport of particles to absorbing traps, which should lead to increased particle absorption.

The main aspects of the simulation algorithm include the following steps:

- System initialization:
 - The number of particles is specified. Their initial positions and spatial distribution are determined by one of the classes responsible for generating the initial population. This class is selected once before the start of the simulation as one of the system parameters.
 - The number of traps is specified. Their initial positions and spatial distribution are also determined by one of the classes responsible for generating traps. This class is selected once before the start of the simulation as one of the system parameters.
 - The trap behavior class is defined, which determines the actions taken when particles enter the traps.
 - The simulation time is specified, which determines the number of algorithm iterations. The number of iterations after which the program saves the system configuration is also specified.
 - The electric field value is specified as a vector. The coordinates of this vector determine the probability of particle displacement in the selected direction.
 - The particle motion algorithm and the interaction method during collisions are specified.
- Particle motion algorithm:
 - At each time step, one of four directions (along the coordinate axes) is randomly selected for each particle.
 - The influence of the electric field is taken into account by increasing the probability of motion in the direction of the field.
 - If two particles attempt to reach the same position, they "repel" each other and remain in their original positions.
 - If more than two particles are involved in a collision, a collision resolution algorithm is used. It first identifies all particles involved in the collision and then determines the final position of each particle.
- Absorption check:

- If a particle enters the coordinates of a trap, the particle is removed from the system.
- A separate class, defined during system initialization, is responsible for the trap's behavior.

Model Implementation

The implementation is written in C++, ensuring high performance.

To simulate random particle movements, a Mersenne Twister random number generator is used. This generator was chosen for its high speed and the quality of its random sequences, allowing it to reliably reproduce the probabilistic displacements of particles. Custom classes for working with hash tables have been implemented, providing fast access to data about particles and traps in space. This structure allows for quick tracking of particles in specific cells, avoiding collisions and ensuring efficient resource management. To speed up simulations, OpenMP parallelization is used. Calculations for experiments in a series are performed in parallel, distributing the load across multithreaded processors and significantly reducing simulation execution time.

Flexible settings for initial system parameters, such as particle density, electric field intensity, and other parameters, have been implemented. These parameters are easily adjusted via configuration files, allowing experimentation with different values without changing the main program code. The implementation allows for easy addition or modification of interaction rules, for example, introducing new types of traps or adjusting the particle motion rules under the influence of the field. Such changes do not require major reworking of the system, allowing for experimentation with new conditions and rules.